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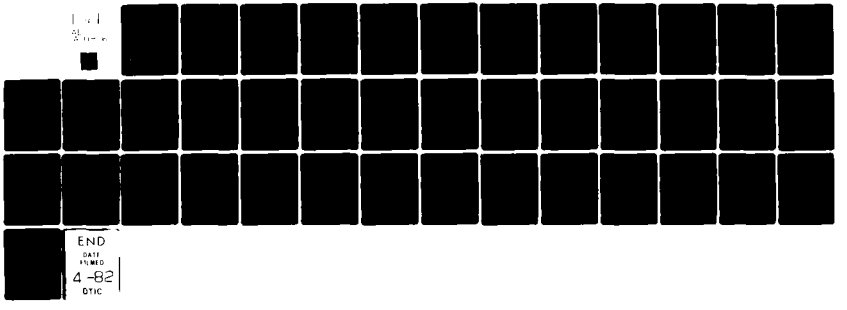

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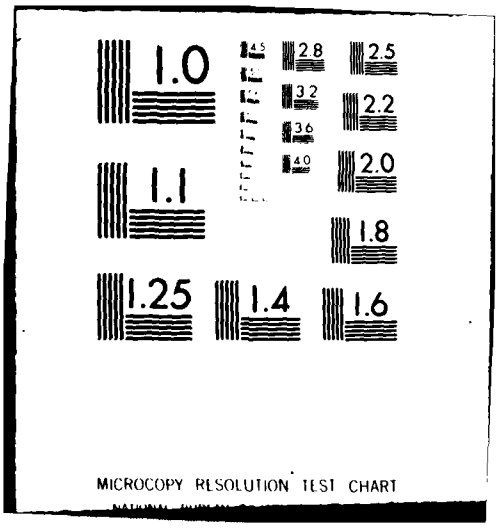
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DIRECT CALCULATION OF THE DERIVATIVES OF THE FREE ENERGY FOR ISING MODELS BY A MODIFIED KADANOFF'S VARIATIONAL METHOD*

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Abstract

We present a systematic procedure for the direct calculation of the free energy and its first and second derivatives for the Ising model in one to three dimensions with a wide class of symmetry properties. This renormalization group method is based on the modified Kadanoff's variational method (MKUM). This method is not only general but also very accurate numerically both near and far from the critical point. Further it includes correction to scaling effects not present in the standard linearized renormalization group treatment. This work describes the techniques and presents some illustrative results for the square lattice and body-centered cubic lattice with nearest neighbor interactions. A full treatment of our results will be given elsewhere.

I. Introduction

In recent years, the position space renormalization group (PSRG) method and its application to phase transitions of various spin models has been widely studied. One important example is Kadanoff's lower bound renormalization group transformation (LBRGT) [1].

In Kadanoff's LBRGT, one has variational parameters in the renormalization group transformation (RGT) equation relating transformed and original unit cell potentials. The optimum variational parameters must be chosen in order to get the best lower bound free energy from the transformed Hamiltonian. Several different methods with different degrees of complexity [2,3,4] have been proposed to determine these variational parameters. One such method is the Modified Kadanoff's Variational Method (MKVM) [3].

In the MKVM, the variational parameter p is determined by minimizing the single cell free energy. This leads to an analytic nonlinear equation for p. In previous papers [3,5], it was found that the MKVM is very accurate for two-valued spin models without external magnetic field in one or two dimensions. It has also been applied to the three dimensional Ising model on a BCC lattice where the derivatives of free energy were calculated by numerical differentiation of the free energy [6].

In this paper, we formulate a systematic procedure to directly calculate the free energy and its first and second derivatives with respect to temperature and external magnetic fields for a wide class of Ising models based on the MKVM. In this way, we avoid the numerical errors arising from numerical differentiation and thus have more accurate derivatives of the free energy for further analysis.

In the application of RG theory to phase transitions, one usually formulates the RGT equations for the coupling constants, then solves them for the fixed point solution(s) and finally expands the RGT equations around the fixed points to find the linearized RGT equation and its eigenvalues and hence critical exponents. Instead of that, we apply the RGT to the Hamiltonian of the given system and calculate the free energy and its first and second derivatives directly. From the behavior of the variational parameters and coupling constants (which tend to larger or smaller values), we can determine the critical point of the given system, which has more direct physical significance than the fixed points. By analyzing the values of the first and second derivatives of the free energy near the critical point, we can determine critical exponents, critical amplitudes and other critical parameters including their less divergent corrections which are of considerable current interest [7,8]. This analysis will be presented elsewhere.

Since the quantities of direct interest here are feee energies and their derivatives, instead of the fixed point and linearized RGT, it is not necessary to carry out the calculation in coupling constant space. In fact, to write a single computer program applicable to many systems with different symmetry properties, it is more convenient to carry out the calculation in cell potential space. This is related to coupling constant space by a linear transformation.

The present paper is organized as follows: In Section II, we derive formulas for free energies and their first and second derivatives with respect to temperature and external magnetic field. These formulas are written in cell potential space instead of coupling constant space. In Section III, we consider some typical systems with various symmetry properties in 1 to 3 space dimensions. We show that we may use very simple criteria to classify all possible spin configurations on a unit cell into different degeneracy groups, each of which corresponds to an independent cell potential. The systems considered are listed in Table I.

We illustrate our formalism in section IV by calculating the free energy and its first and second derivatives with respect to temperature and external magnetic field for Ising models on two dimensional square and three dimensional BCC lattices. Our results are compared with exact [9,10] and series expansion values [11,12] and are shown in Fig. 1 and 2. In section V, we give a brief discussion of possible extensions our method.

II. General Formalism

Let us consider N Ising spins σ_i ($=\pm 1$) on a general d dimensional lattice, which interact with each other via a Hamiltonian of the form [1]:

$$\beta H(\sigma_1, \sigma_2, \cdots \sigma_N) = - \sum_{R'} v_{R'}(\sigma_{R'}) \quad , \tag{1}$$

where $\sum_{R'}$ is a sum over d dimensional hypercube unit cells of the lattice. $\sigma_{R'} = \{\sigma_1, \cdots \sigma_Z\}$ with $Z=2^d$ are spins at the corners of the unit cell R' and $v(\sigma_{R'})$ is the interaction potential of the spins $\sigma_{R'}$ within the unit cell R'. After a Kadanoff's LBRGT, the transformed Hamiltonian for N' Ising spins μ_i ($=\pm 1$) on lattice with double lattice spacing has the same form as Eq. (1), i.e.:

$$\beta H'(\mu_1, \mu_2, \cdots \mu_{N'}) = - \sum_{R} v'_R(\mu_R) \quad , \tag{2}$$

where N' is the number of spins on the new lattice (N'=N/Z), $v_{R'}(\mu_R)$ is the interaction potential for the Ising spin $\mu_R=\{\mu_1, \cdots \mu_Z\}$ on a hypercube unit cell R with doubled the original lattice spacing., and $v_{R'}$ is related to $v_R(\sigma_{R'})$ by the RGT equation (hereafter we will drop the subscripts on $v_{R'}(\sigma_{R'})$ and $v_R(\mu_R)$:

$$\exp[v'(\mu)] = \sum_{\sigma_1, \cdots \sigma_Z} \exp\left[Z v(\sigma) + p \sum_{i=1}^{Z} \mu_i \sigma_i - u(\sigma, p)\right] \quad , \tag{3}$$

with u (σ,p) given by:

$$u(\sigma, p) = \ln(e^{ps_1} + e^{-ps_1}) \quad , \tag{4}$$

where $s_1 = \sum_{i=1}^{Z}$ and p is a parameter. It follows from Eq. (3) and (4) that $v'(\mu)$ and $v(\sigma)$ have the same symmetry properties with respect to the point group transformation of spins within the hypercube unit cell. Thus v and v' can be expressed in terms of the same invariant functions of Ising spins on the hypercube unit cell:

$$v(\sigma) = \sum_{i=0}^{\ell} K_i g_i(\sigma) \quad , \tag{5a}$$

$$v'(\mu) = \sum_{i=0}^{\ell} K'_i g_i(\mu) \quad , \tag{5b}$$

where $g_0=(\sigma)=g_0(\mu)=1$. The other g_i are defined and discussed in Appendix A. Let $\vec{K}=(K_0,K_1,---K_\ell)$ and $\vec{K}'=(K_0',K_1',---K_\ell')$ denote vectors of the coupling constants. Then Eq. (3) may be considered as a transformation of the coupling constants:

$$\vec{K}' = \vec{F}(\vec{K}, p) \quad . \tag{6}$$

For Z Ising spins on a hypercube unit cell, there are 2^Z possible spin configurations and thus 2^Z possible hypercube cell potential $v'(\mu)$. However, many $v'(\mu)$ are equal due to the symmetries of the spins on a unit cell. In fact, the number of independent $v'(\mu)$ is the same as the number of independent coupling constants in Eq. (5), ie $\ell+1$. Let $\vec{v}'$ denote the vector of these independent cell potentials $(v_1,v_2,---v_{\ell+1})$. Then v' is related to $K'=(K_0',K_1',---K_\ell')$ by the linear transformation of the $(\ell+1)$ x $(\ell+1)$ matrix T:

$$(v_1', v_2', \cdots v_{\ell+1}') = (K_0', K_1', \cdots K_\ell')T \quad , \tag{7}$$

or briefly denoted as:

$$\vec{v}' = \vec{K}'T \quad . \tag{8}$$

T can be calculated from Eq. (5).

We also have the inverse transformation

$$\vec{K}' = \vec{v}'T^{-1} \tag{9}$$

where T^{-1} T=I.

Now the free energy calculated from $H'(\mu_1,--\mu_{N'})$ is always a lower bound for free energy calculated from $H(\sigma_1,\sigma_2,--\sigma_N)$ and we must vary p to obtain the optimum lower bound free energy. In the MKVM, the variational parameter p is determined by minimizing the single cell free energy. This leads to the nonlinear equation:

$$\frac{\sum_{\mu_1,\cdots\mu_Z} \frac{\partial v'}{\partial p} \exp[v'(\mu)]}{\sum_{\mu_1,\cdots\mu_Z} \exp[v'(\mu)]} = 0 \quad , \tag{10}$$

which is solved at each iterative step to determine P. From Eq. (3), (4) and (10), it is easy to show that Eq. (10) may be rewritten as:

$$\frac{\sum_{i=1}^{p+1} D_i \exp(z v_i) \frac{d}{dp} F(S_{1,i}; P)}{\sum_{i=1}^{p+1} D_i \exp(z v_i) F(S_{1,i}; P)} = 0 , \tag{11}$$

With $F(S_{1,i}, p)$ given by

$$F(S_{1,i}; P) = (2\cosh p)^z / 2\cosh(p S_{1,i}) , \tag{12}$$

Where $S_{1,i}$ is $\sum_{j=1}^{z} \sigma_j$ evaluated at the i th degeneracy group. Di and v_i are the number of elements and cell potential for the i th degeneracy group respectively.

To begin with, we use $v_{R'}$ ($\sigma_{R'}$) of Eq. (1) as $v(\sigma)$ in the right hand side of Eq. (3) with p given by Eq. (11) and calculate the cell potential $v'(\mu)$ from Eq. (3). This constitutes the first step of the RG transformation. We then use $v'(\mu)$ thus obtained as input in the same procedure to calculate the transformed potential $v''(\mu)$. This RG transformation is iterated further so that a series of cell potentials $v'(\mu)$, $v''(\mu)$,---$v^{(\alpha)}(\mu)$ (and hence coupling constants K', K",---$K^{(\alpha)}$ and the corresponding variational parameters p',p",---$p^{(\alpha)}$) are obtained. In this step by step RG transformation $K_i(\alpha)$ for $i \geq 1$ and $p^{(\alpha)}$ tend to diminish to zero with increasing α when the system is above the critical temperature and tend to grow when the system is below the critical temperature. Thus, after a large number, say α, of RG transformations, β times the free energy per spin for the original lattice may be approximated by:

$$f^{(\alpha)} \simeq -\frac{1}{2^\alpha}\left(K_0^{(\alpha)} + \ln 2\right) , \tag{13a}$$

for $T > T_c$ (or $\beta < \beta_c = \frac{1}{kT_c}$) and

$$f^{(\alpha)} = -\frac{1}{Z^{\alpha}}\left[K_0^{(\alpha)} + \sum_{i=1}^{\ell} K_i^{(\alpha)} g_i(\vec{\sigma}_0) + \ln(2)\right], \tag{13b}$$

for $T < T_c$ (or $\beta > \beta_c$), where $\vec{\sigma}_0$ is the spin configuration at T=0.

To calculate the internal energy and spontaneous magnetization of the system, we must take the first derivative of $f^{(\alpha)}$ with respect to β and $h(=\beta B)$ respectively. Let q denote either β or h. By the chain rule, it is easy to see from Eq. (13) that:

$$\frac{\delta f^{(\alpha)}}{\delta q} = -\frac{\delta \vec{K}^0}{\delta q}\cdot\frac{\delta \vec{K}^{(1)}}{\delta \vec{K}^0}\cdots\frac{\delta \vec{K}^{(m)}}{\delta \vec{K}^{(m-1)}}\cdots\frac{\delta \vec{K}^{(\alpha)}}{\delta \vec{K}^{(\alpha-1)}}\frac{1}{Z^{\alpha}}\vec{C}, \tag{14}$$

where

$$\vec{C} = (1, 0, \cdots 0)^T, \tag{15a}$$

for $T > T_c$ and

$$\vec{C} = (1, g_1(\vec{\sigma}_0), g_2(\vec{\sigma}_0), \cdots g_\ell(\vec{\sigma}_0))^T, \tag{15b}$$

for $T < T_c$.

It will become clear later that in order to deal with systems with different symmetry properties in a unified way, it is convenient to carry out the calculation in the cell potential space $v^{(\alpha)}(\mu)$ instead of the coupling constant space $K^{(\alpha)}$. From Eq. (8) and (9), we have

$$\frac{\delta \vec{K}^{(m)}}{\delta \vec{K}^{(m-1)}} = T\frac{\delta \vec{v}^{(m)}}{\delta \vec{v}^{(m-1)}}T^{-1}, \tag{16a}$$

$$\frac{\delta \vec{K}_0}{\delta q} = \frac{\delta \vec{v}^{\,0}}{\delta q}T^{-1}. \tag{16b}$$

Thus Eq. (14) may be rewritten as:

$$\frac{\delta f^{(\alpha)}}{\delta q} = -\frac{\delta \vec{v}^{\,0}}{\delta q}\cdot\frac{\delta \vec{v}^{(1)}}{\delta \vec{v}^{0}}\cdots\frac{\delta \vec{v}^{(m)}}{\delta \vec{v}^{(m-1)}}\cdots\frac{\delta \vec{v}^{(\alpha)}}{\delta \vec{v}^{(\alpha-1)}}\cdot\frac{1}{Z^{\alpha}}T^{-1}\vec{C}. \tag{17}$$

In Appendix B, we derive very simple general formulas for $T\vec{C}$ that allow us to avoid explicitly calculating the matrix T.

It should be noted that for q=h in Eq. (14), $\vec{K}^{(m)}$ for m=1,---,α must include all odd spin coupling constants even if we evaluate the row vector $\frac{\delta \vec{K}^{0}}{\delta h}$ and matrix $\frac{\delta \vec{K}^{(m)}}{\delta \vec{K}^{(m-1)}}$ at points where the odd spin coupling constants vanish These points are equivalent to the points in the cell potential space with $\upsilon(\sigma_1,\ldots\sigma_z) = \upsilon(-\sigma_1,\ldots-\sigma_z)$. Thus to evaluate the spontaneous magnetization in cell potential space, we must consider $\upsilon(\sigma_1, \sigma_2,\ldots\sigma_z)$ and $\upsilon(-\sigma_1, -\sigma_2,\ldots-\sigma_z)$ as independent cell potentials.

To calculate the specific heat and susceptibility of the system, we must take the second derivative of $f^{(\alpha)}$ with respect to β and h. From Eq. (17), it follows that:

$$\begin{aligned}\frac{\delta^2 f^{(\alpha)}}{\delta g^2} = -\Bigg\{ & \frac{\delta^2 \vec{\upsilon}^{0}}{\delta g^2}\cdot\frac{\delta \vec{\upsilon}^{(1)}}{\delta \vec{\upsilon}^{0}}\cdots\frac{\delta \vec{\upsilon}^{(m)}}{\delta \vec{\upsilon}^{(m-1)}}\cdots\frac{\delta \vec{\upsilon}^{(\alpha)}}{\delta \vec{\upsilon}^{(\alpha-1)}} \\ & + \frac{\delta \vec{\upsilon}^{0}}{\delta g}\cdot\frac{\delta^2 \vec{\upsilon}^{1}}{\delta g\,\delta \vec{\upsilon}^{0}}\cdots\frac{\delta \vec{\upsilon}^{(m)}}{\delta \vec{\upsilon}^{(m-1)}}\cdots\frac{\delta \vec{\upsilon}^{(\alpha)}}{\delta \vec{\upsilon}^{(\alpha-1)}} \\ & + \cdots \\ & + \frac{\delta \vec{\upsilon}^{0}}{\delta g}\cdot\frac{\delta \vec{\upsilon}^{(1)}}{\delta \upsilon^{0}}\cdots\frac{\delta}{\delta g}\frac{\delta \vec{\upsilon}^{(m)}}{\delta \vec{\upsilon}^{(m-1)}}\cdots\frac{\delta \vec{\upsilon}^{(\alpha)}}{\delta \vec{\upsilon}^{(\alpha-1)}} \\ & + \cdots \\ & \vdots \\ & + \frac{\delta \vec{\upsilon}^{0}}{\delta g}\cdot\frac{\delta \vec{\upsilon}^{(1)}}{\delta \vec{\upsilon}^{0}}\cdots\frac{\delta \vec{\upsilon}^{(m)}}{\delta \vec{\upsilon}^{(m-1)}}\cdots\frac{\delta}{\delta g}\frac{\delta \vec{\upsilon}^{(\alpha)}}{\delta \vec{\upsilon}^{(\alpha-1)}}\Bigg\}\frac{1}{z^{\alpha}}T^{-1}\vec{C}, \end{aligned} \tag{18}$$

By the chain rule $\frac{\delta}{\delta g}\frac{\delta \vec{\upsilon}^{(m)}}{\delta \vec{\upsilon}^{(m-1)}}$ for $m=1,\cdots\alpha$ is further given by:

$$\frac{\delta}{\delta g}\frac{\delta \vec{\upsilon}^{(m)}}{\delta \vec{\upsilon}^{(m-1)}} = \frac{\delta \vec{\upsilon}^{0}}{\delta g}\cdot\frac{\delta \vec{\upsilon}^{(1)}}{\delta \vec{\upsilon}^{0}}\cdots\frac{\delta}{\delta \vec{\upsilon}^{(m-1)}}\frac{\delta \vec{\upsilon}^{(m)}}{\delta \vec{\upsilon}^{(m-1)}}, \tag{19}$$

Thus to calculate $\frac{\delta f^{(\ell)}}{\delta \beta}$ and $\frac{\delta^2 f^{(\ell)}}{\delta \beta^2}$, we must

evaluate $\frac{\delta \vec{v}^0}{\delta \beta}$, $\frac{\delta^2 \vec{v}^0}{\delta \beta^2}$, $\frac{\delta v_j^{(m)}}{\delta v_i^{(m-1)}}$ and $\frac{\delta}{\delta v_k^{(m-1)}} \frac{\delta v_j^{(m)}}{\delta v_i^{(m-1)}}$

for i, j, k = 1, ---, ℓ+1. It is straightforward to calculate the first two quantities from the initial cell potential of Eq. (1). From Eq. (3), we have

$$v_j^{(m)} = \ln\left[\sum_{\sigma} \exp\left(z v^{(m-1)}(\sigma) + p \sum_{k=1}^{z} \mu_k \sigma_k - u(\sigma, p)\right)\right], \tag{20}$$

where $(\mu_1, \text{--}\mu_z)$ is one of the spin configuration belonging to the j th degeneracy group and $u(\sigma,p)$ is given by Eq. (4). The variational parameter p of Eq. (20) is essentially determined by the initial cell potentials $v^{(m-1)}$. This fact must be taken into account in the calculation of $\frac{\delta v_j^{(m)}}{\delta v_i^{(m-1)}}$. Thus we have

$$\frac{\delta v_j^{(m)}}{\delta v_i^{(m-1)}} \equiv \left(\frac{\delta \vec{v}^{(m)}}{\delta \vec{v}^{(m-1)}} \right)_{ij} = \left(\frac{\partial v_j^{(m)}}{\partial v_i^{(m-1)}}\right)_p + \left(\frac{\partial v_j^{(m)}}{\partial p}\right)\left(\frac{\partial p}{\partial v_i^{(m-1)}}\right), \tag{21}$$

Where

$$\left(\frac{\partial v_j^{(m)}}{\partial v_i^{(m-1)}}\right)_p = \frac{z \sum_{\sigma}' \exp\left[z v^{(m-1)}(\sigma) + p \sum_{k=1}^{z} \mu_k \sigma_k - u(\sigma,p)\right]}{\sum_{\sigma} \exp\left[z v^{(m-1)}(\sigma) + p \sum_{k=1}^{z} \mu_k \sigma_k - u(\sigma,p)\right]}, \tag{22}$$

$$\frac{\partial v_j^{(m)}}{\partial p} = \frac{\sum_{\sigma} \exp\left[z v^{(m-1)}(\sigma) + p \sum_{k=1}^{z} \mu_k \sigma_k - u(\sigma,p)\right]\left(\sum_{k=1}^{z} \mu_k \sigma_k - \frac{\partial}{\partial p} u\right)}{\sum_{\sigma} \exp\left[z v^{(m-1)}(\sigma) + p \sum_{k=1}^{z} \mu_k \sigma_k - u(\sigma,p)\right]}, \tag{23}$$

and

$$\frac{\partial p}{\partial v_i^{(m-1)}} = - \frac{z D_i \exp\left(z v_i^{(m-1)}\right) \frac{d}{dp} F(S_1, i; p)}{\sum_{k=1}^{\ell+1} D_k \exp\left(z v_k^{(m-1)}\right) \frac{d^2}{dp^2} F(S_1, i; p)}, \tag{24}$$

where $F(S_1,_i;p)$ is given by Eq. (12). In Eq. (22), $\sum'$ is a sum over all configurations of σ corresponding to the cell potential $v_i^{(m-1)}(\sigma)$. Eq. (24) is derived from Eq. (11) and the notation is the same as that of Eq. (11).

From Eq. (21), it follows that

$$\frac{\delta^2 v_j^{(m)}}{\delta v_k^{(m-1)} \delta v_i^{(m-1)}} = \left(\frac{\partial v_j^{(m)}}{\partial v_k^{(m-1)} \partial v_i^{(m-1)}}\right)_p + \frac{\partial v_j^{(m)}}{\partial v_k^{(m-1)} \partial p} \frac{\partial p}{\partial v_i^{(m-1)}}$$
$$+ \frac{\partial v_j^{(m)}}{\partial p} \cdot \frac{\partial^2 p}{\partial v_k^{(m-1)} \partial v_i^{(m-1)}} + \left[\frac{\partial v_j^{(m)}}{\partial p \partial v_i^{(m-1)}}\right.$$
$$\left. + \frac{\partial^2 v_j^{(m)}}{\partial p^2} \cdot \frac{\partial p}{\partial v_i^{(m-1)}} + \frac{\partial v_j^{(m)}}{\partial p} \cdot \frac{\partial}{\partial p} \frac{\partial p}{\partial v_i^{(m-1)}}\right] \frac{\partial p}{\partial v_k^{(m-1)}} . \qquad (25)$$

It is straightforward to derive equations for the partial derivatives on the right hand side of Eq. (25). They are very involved so we do not report them here. It is obvious that Eq. (25) is symmetric with respect to the indices K and i. We have used this fact to check our expressions for the right hand side of Eq. (25).

This completes our formulation of the equations for the direct calculation of the first and second derivatives of the free energy.

III. Symmetry Properties

In order to carry out the configuration sum Σ' in Eq. (22) and also the equations for the partial derivatives with respect to $v_K^{(m-1)}$, $v_i^{(m-1)}$ on the right side of Eq. (25), we must establish the correspondence between spin configurations $(\sigma_1, --\sigma_z)$ and the independent cell potentials $v_i(\sigma_1, --\sigma_z)$. That is, we must classify the 2^z possible spin configurations into different groups, such that all configurations of the same group have the same cell potential $v_i(\sigma_1,---\sigma_z)$, where i runs from 1 to $\ell+1$. This correspondence depends on the space dimension and symmetry properties of the system. However, we can establish very simple general criteria for the purpose of such configuration classification.

In Appendix A, we list invariant functions for certain systems in one to three dimensions. We also list the relations between invariants of a given system. From such relations, it is easy to see that all invariants for a given system may be expressed in terms of certain basic invariants. These are also given Table I. Thus by Eq. (5), any cell potential $v(\sigma_1,---\sigma_z)$ can be expressed as a function of these basic invariants. So we may use these basic invariants as criteria to classify the spin configurations. The generation of all possible configurations and their classification into different groups based on their basic invariants may be carried out simply by computer. This scheme is briefly described in Appendix B.

In Table I, we also list the values of $\ell+1$ and possible applications of the considered models.

Table 1. Basic Invariants and possible applications for the considered models.

Note that the definition of g_1 (see Appendix A) may differ from case to case.

Model	Dimension	Basic Invariants	$\ell+1$	application[a]
S_1	1	g_1	3	
S_2	2	g_2	5	Isotropic SQ lattice with nn interaction only.
S_3	2	g_1, g_2	6	Isotropic SQ lattice with nn, nnn and 4 spin interactions.
S_4	2	g_1, g_2, g_3	7	Anisotropic SQ lattice with nn, nnn, and 4 spin interactions.
S_5	2	g_1, g_2	9	Triangular lattice with nn and nnn interactions.
S_6	3	g_1	9	Isotropic BCC lattice with nn interaction only.
S_7	3	g_1, g_2, g_3	22	Isotropic SC lattice with all possible even spin interactions within the primitive unit cell.
S_8	3	g_1, g_2, g_3, g_4, g_5	34	Anisotropic SC (tetragonal) lattice. Crossover from d=2 to d=3.
S_9	3	g_1, g_2, g_3, g_4, g_5	46	Isotropic FCC lattice will all possible even spin interactions within the primitive unit cell.

a. nn = nearest neighbor, nnn = next nearest neighbor.

IV. An Example: Permulation Symmetry

In this section, we apply the formalism developed in the previous sections to an Ising model with isotropic nearest neighbor interactions on 1 dimensional, 2 dimensional square, and 3 dimensional body-centered cubic lattices. The Hamiltonian in these cases may be written as:

$$\beta H = -K \sum_{<ij>} \sigma_i \sigma_j - h \sum_i \sigma_i \equiv - \sum_R v_R \,, \tag{26a}$$

$$v_R = K \sigma_c (\sigma_1 + \cdots \sigma_z) + \frac{h}{z} (\sigma_1 + \cdots \sigma_z) + h \sigma_c \,, \tag{26b}$$

where R is a unit cell with one spin σ_c in the center, Z spins $\sigma_1, \cdots \sigma_z$ at the corners and the factor $\beta (= \frac{1}{kT})$ has already been included in K and h. Performing a decimation calculation which sums over the central spin in each cell, we obtain an effective Hamiltonian for the remaining spins. The resulting cell potential is

$$v_{eff,R} = \frac{h}{z} (\sigma_1 + \cdots + \sigma_z) + \ln 2 \cosh \left(h + K (\sigma_1 + \cdots + \sigma_z) \right) \,, \tag{27}$$

Eq. (27) has permutation symmetry with respect to σ_1, σ_2, $\cdots \sigma_z$ and thus according to Appendix A can be classified as S1, S2, or S6 for d equals 1, 2 or 3 respectively. We can use $g_1 = \sigma_1 + \cdots + \sigma_z$ as the basic invariant to classify the 2^z possible configurations of $\sigma_1, \cdots \sigma_z$ into different degeneracy groups, each of which corresponds to the same cell potential. We then use $v_{eff,R}$ of Eq. (7) as $\vec{v}_0$ in Sec. 2 to calculate the free energy per spin and its first and second derivatives with respect to k and h. We must divide all these quantities by a factor 2 because Eq. (27) was obtained after a decimation calculation. The results for d=1 agree extremely well with the exact results

obtained by transfer matrix method [9]. These results also provide a check on our computer program.

A few results for d=2 and 3 are shown in Fig. 1 and Fig. 2 respectively. Fig. 1b and Fig. 1c should be compared with Fig. 6 and 7 in Kadanoff et al.'s paper [1]. Their results were obtained by numerical differentiation for the free energy and thus involve more numerical error than the present work.

In future work, we will present the results of this method applied to several models with different symmetry properties. Preliminary analysis indicates that we obtain very accurate values both close to and far from the transition temperature, as is clear from Fig. 1 and 2. The application of this method near the transition temperature is of particular interest since it allows an evaluation of correction to scaling effects due to nonlinear terms and all the (linearized renormalization group) eigenvalues.

V. Discussion

From the previous sections, it is clear that to calculate the free energy and its derivatives for given model. It is sufficient to use the basic invariants of such model and not necessary to use the relations among all invariants, i.e. the even numbered equations of Appendix A. For a given system, to obtain the former is much easier than the latter. However, if we desire to calculate the flow of the coupling constants (k_1, k_2, --k_ℓ) in parameter space as the step by step RG transformation is carried out, we may use the even numbered equations of Appendix A to calculate the $(\ell+1) \times (\ell+1)$ matrix T and hence T^{-1} of Eq. (8) and (9) respectively.

The method used in this paper may be easily extended and applied to systems with symmetry properties different from those listed in Table I. In particular, we may combine the ideas of this paper and our previous paper [14] to calculate derivatives of free energy for antiferromagnetic systems.

Figure Captions

Fig. 1. Derivatives of the free energy for the Ising Model on the SQ lattice. (a) $-\frac{\delta f}{\delta k}$ as function of K. (b) $-\frac{\delta^2 f}{\delta K^2}$ as function of K. (c) M^8 as function of K, where $M = -\frac{\delta f}{\delta h}$. (d) $\ln \chi$ as a function of k, where $\chi = -K\frac{\delta^2 f}{\delta^2 h}$.

The solid curves in Fig. 1a, 1b and 1c represent Onsager [9] or Yang's [10] exact solution. The solid curve in Fig. 1d is obtained from high temperature [12] and low temperature [11] serious expansion for $K \leq 0.4407$ and $K > 0.4407$ respectively.

Fig. 2. Derivatives of the free energy for the Ising model on the BCC lattice. (a) $-\frac{\delta f}{\delta k}$ as function of K. (b) $-\frac{\delta^2 f}{\delta k^2}$ as function of K. (c) M as function of k, where $M = -\frac{\delta f}{\delta h}$. (d) $\ln \chi$ as a function of k, where $\chi = -k\frac{\delta^2 f}{\delta^2 h}$. The solid curves are obtained from high temperature [12] or low temperature [11] series expansion for $K \leq 0.1574$ respectively.

Fig. A1. Location of Ising spin σ_1, σ_2 on one dimensional unit cell.

Fig. A2. Location of Ising spins σ_1, σ_2, σ_3, σ_4 on the two dimensional unit cell. $\vec{a}$ and $\vec{b}$ are the primitive translation vectors and α is the angle between them.

Fig. A3. Location of Ising spins σ_1, σ_2, ---σ_8 on the three dimensional unit cell. $\vec{a}$, $\vec{b}$, and $\vec{c}$ are the primitive translation vector and α, β, γ are the angles between them.

APPENDIX A

Symmetry Properties and Invariant Functions for Ising Spins on Hypercube Unit Cell.

The location of the z ($=2^d$) Ising spins on a hypercube unit cell are shown in Fig. A1, Fig. A2 and Fig. A3 for d=1, 2 and 3 respectively. We shall use K_{ij} to denote the two-spin coupling constant between σ_i and σ_j which appears on the right hand side of Eq. (5).

Now we consider the following possible systems and write down the invariant functions on the right hand side of Eq. (5) for them.

S1 d=1

$$g_1 = \sigma_1+\sigma_2,$$
$$g_2 = \sigma_1\sigma_2. \qquad \text{(A1)}$$

They satisfy the relation:

$$g_2^2 = g_1^2/2 - 1 . \qquad \text{(A2)}$$

S2 d=2 $\upsilon(\sigma_1,--\sigma_4)$ has permutation symmetry.

$$g_1 = \sigma_1+\sigma_2+\sigma_3+\sigma_4,$$
$$g_2 = \sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_1+\sigma_1\sigma_3+\sigma_2\sigma_4,$$
$$g_3 = \sigma_1\sigma_2\sigma_3+\sigma_2\sigma_3\sigma_4+\sigma_3\sigma_4\sigma_1+\sigma_4\sigma_1\sigma_2,$$
$$g_4 = \sigma_1\sigma_2\sigma_3\sigma_4. \qquad \text{(A3)}$$

They satisfy the relations

$$g_2 = g_1^2/2 - 2,$$
$$g_3 = [g_1g_2 - 3g_1]/3,$$
$$g_4 = [g_1g_3 - 2g_2]/4. \qquad \text{(A4)}$$

S3 d=2 $\upsilon(\sigma_1,--\sigma_4)$ has rotation, reflection and inversion symmetries. $K_{12}=K_{23}=K_{34}=K_{41}$, $K_{13}=K_{24}$ but $K_{12} \neq K_{13}$. For the unit cell of Fig. A2, $|\vec{a}| = |\vec{b}|$,

$$g_1 = \sigma_1+\sigma_2+\sigma_3+\sigma_4,$$
$$g_2 = \sigma_1\sigma_3+\sigma_2\sigma_4,$$
$$g_3 = \sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_1,$$
$$g_4 =\sigma_1\sigma_2\sigma_3+\sigma_2\sigma_3\sigma_4+\sigma_3\sigma_4\sigma_1+\sigma_4\sigma_1\sigma_2,$$
$$g_5 = \sigma_1\sigma_2\sigma_3\sigma_4, \qquad \text{(A5)}$$

They satisfy the relations

$$g_3 = g_1^{\,2}/2 - g_2 - 2,$$
$$g_4 = g_1g_2 - g_1$$
$$g_5 = g_2^{\,2}/2 - 1. \qquad \text{(A6)}$$

S4 d=2 $v(\sigma_1,--\sigma_4)$ has reflection and inversion symmetries.

$K_{12}=K_{34}$, $K_{23}=K_{41}$, $K_{12}\neq K_{23}$.

$K_{13}=K_{24}$. For the unit cell of Fig. A2, $\vec{a} \neq \vec{b}$, $\alpha=90°$

$$g_1 = \sigma_1+\sigma_2+\sigma_3+\sigma_4,$$
$$g_2 = \sigma_1\sigma_3+\sigma_2\sigma_4,$$
$$g_3 = \sigma_1\sigma_2+\sigma_3\sigma_4,$$
$$g_4 = \sigma_1\sigma_4 + \sigma_2\sigma_3,$$
$$g_5 = \sigma_1\sigma_2\sigma_3 + \sigma_2\sigma_3\sigma_4 + \sigma_3\sigma_4\sigma_1 + \sigma_4\sigma_1\sigma_2,$$
$$g_6 = \sigma_1\sigma_2\sigma_3\sigma_4 \qquad \text{(A7)}$$

They satisfy the relations:

$$g_4^2 = g_1^2/2 - g_2 - g_3 - 2,$$
$$g_5 = g_1g_2 - 1$$
$$g_6 = g_2^2 - 1 \qquad \text{(A8)}$$

S5 d=2 $v(\sigma_1,--\sigma_4)$ has inversion symmetry.

$K_{12}=K_{23}=K_{34}=K_{41}$, $K_{13} \neq K_{24}$. for the unit cell of Fig. A2, $|\vec{a}| = |\vec{b}|$, $\alpha = 60^o$.

$$g_1=\sigma_1+\sigma_3,$$

$$g_2=\sigma_2+\sigma_4,$$

$$g_3=\sigma_1\sigma_3,$$

$$g_4=\sigma_2\sigma_4,$$

$$g_5=\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_1,$$

$$g_6=\sigma_1\sigma_2\sigma_3+\sigma_1\sigma_3\sigma_4,$$

$$g_7=\sigma_1\sigma_2\sigma_4+\sigma_2\sigma_3\sigma_4,$$

$$g_8=\sigma_1\sigma_2\sigma_3\sigma_4. \qquad \text{(A9)}$$

They satisfy the relations:

$$g_3=g_1^2/2-1,$$

$$g_4=g_2^2/2-1,$$

$$g_5=g_1g_2,$$

$$g_6=g_2g_3,$$

$$g_7=g_1g_4,$$

$$g_8=g_3g_4 \qquad \text{(A10)}$$

S6 d=3 $v(\sigma_1,--\sigma_8)$ has permutation symmetry.

Let g_i denote the sum of all possible products of i different σ's. g_i for i=1,..8 are the basic invariants of the permutation group. It is easy to show that g_i satisfy for relation:

$$g_1=\sigma_1+\sigma_2+--+\sigma_8 \quad , \tag{A11}$$

$$g_{i+1}=[g_1 g_i - (8-i+1)\, g_{i-1}]\,/_{(i+1)}, \tag{A12}$$

for i=1,...7. Thus each g_i may be expressed in terms of g_1.

S7 d=3 $v(\sigma_1,--\sigma_8)$ of Eq. (5) has symmetry properties of the simple cubic unit cell, i.e. O_h point group.

$g_1=\sigma_1+\sigma_2+\sigma_3+--+\sigma_8$,

$g_2=\sigma_1\sigma_2+---$ (12 terms),

$g_3=\sigma_1\sigma_7+---$ (4 terms),

$g_4=\sigma_1\sigma_3+---$ (12 terms),

$g_5=\sigma_1\sigma_2\sigma_3\sigma_4+---$ (6 terms),

$g_6=\sigma_1\sigma_2\sigma_3\sigma_8+---$ (24 terms),

$g_7=\sigma_1\sigma_2\sigma_3\sigma_6+---$ (8 terms),

$g_8=\sigma_1\sigma_2\sigma_3\sigma_7+---$ (24 terms),

$g_9=\sigma_1\sigma_2\sigma_7\sigma_8+---$ (6 terms),

$g_{10}=\sigma_1\sigma_3\sigma_6\sigma_8+---$ (2 terms),

$g_{11}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6+---$(12 terms),

$g_{12}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_7+---$(12 terms),

$g_{13}=\sigma_1\sigma_2\sigma_3\sigma_5\sigma_7\sigma_8+---$(4 terms),

$g_{14}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7\sigma_8$(1 term),

$g_{15}=\sigma_1\sigma_2\sigma_3+---$ (24 terms),

$g_{16}=\sigma_1\sigma_2\sigma_7+---$ (24 terms),

$g_{17}=\sigma_1\sigma_3\sigma_6+---$ (8 terms),

$g_{18}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5+---$ (24 terms),

$$g_{19}=\sigma_1\sigma_2\sigma_3\sigma_7\sigma_8+\text{---} \quad \text{(24 terms)},$$
$$g_{20}=\sigma_1\sigma_3\sigma_4\sigma_6\sigma_8+\text{---} \quad \text{(8 terms)},$$
$$g_{21}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7+\text{---} \quad \text{(8 terms)}, \qquad \text{(A13)}$$

Where, in order to save space, only one typical term for each invariant is written. It is easy to show that the g_i of Eq. (A13) are related to each other by the equations:

$$g_4= g_1^2/2-g_2-g_3,$$
$$g_6= g_3g_4-2g_2,$$
$$g_8=g_2g_3-2g_4,$$
$$g_9=g_3^2/2-2,$$
$$g_5=g_2^2/2-6-2g_4-g_8-g_9,$$
$$g_7=(g_2g_4-4g_2-6g_3-2g_6)/3,$$
$$g_{10}=g_4^2/6-2-\tfrac{2}{3}g_4-g_5/3-g_8/3-g_9/3,$$
$$g_{14}=g_{10}^2/2-1,$$
$$g_{11}=g_2g_{14},$$
$$g_{12}=g_3g_{14},$$
$$g_{13}=g_4g_{14},$$
$$g_{16}=g_1g_3-g_1,$$
$$g_{15}=(g_1g_2-3g_1-g_{16})/2,$$
$$g_{17}=(g_1g_4-3g_1-g_{15}-g_{16})/3,$$
$$g_{18}=g_{14}g_{15},$$
$$g_{19}=g_{14}g_{16}, \qquad \text{(A14)}$$
$$g_{20}=g_{14}g_{17},$$
$$g_{21}=g_{14}g_1$$

S8 d=3 $\upsilon(\sigma_1, \sigma_2, --\sigma_8)$ of Eq (5) has symmetry properties of the tetragonal unit cell. For the unit cell of Fig. A3, $|\vec{a}| = |\vec{b}| \neq |\vec{c}|$, $\alpha = \beta = \gamma = 90^{o}$.

$g_1=\sigma_1+\sigma_2+\sigma_3+\sigma_4+\sigma_5+\sigma_6+\sigma_7+\sigma_8$,

$g_2=\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_1+\sigma_5\sigma_6+\sigma_6\sigma_7+\sigma_7\sigma_8+\sigma_8\sigma_1$,

$g_3=\sigma_1\sigma_5+\sigma_2\sigma_6+\sigma_3\sigma_7+\sigma_4\sigma_8$,

$g_4=\sigma_1\sigma_7+\sigma_2\sigma_8+\sigma_3\sigma_5+\sigma_4\sigma_6$,

$g_5=\sigma_1\sigma_3+\sigma_2\sigma_4+\sigma_5\sigma_7+\sigma_6\sigma_8$,

$g_6=\sigma_1\sigma_6+\sigma_2\sigma_5+\sigma_2\sigma_7+\sigma_3\sigma_6+\sigma_3\sigma_8+\sigma_4\sigma_7+\sigma_1\sigma_8+\sigma_4\sigma_5$,

$g_7=\sigma_1\sigma_2\sigma_3\sigma_4+\sigma_5\sigma_6\sigma_7\sigma_8$

$g_8=\sigma_1\sigma_2\sigma_6\sigma_5+\sigma_2\sigma_3\sigma_7\sigma_6+\sigma_3\sigma_4\sigma_8\sigma_7+\sigma_1\sigma_4\sigma_5\sigma_8$,

$g_9=\sigma_1\sigma_2\sigma_3\sigma_8+$--- (8 terms)

$g_{10}=\sigma_1\sigma_2\sigma_6\sigma_8+$--- (16 terms)

$g_{11}=\sigma_1\sigma_2\sigma_3\sigma_6+$--- (8 terms)

$g_{12}=\sigma_1\sigma_2\sigma_3\sigma_7+$--- (16 terms)

$g_{13}=\sigma_1\sigma_2\sigma_6\sigma_7+$--- (8 terms)

$g_{14}=\sigma_1\sigma_2\sigma_7\sigma_8+$--- (4 terms)

$g_{15}=\sigma_1\sigma_5\sigma_3\sigma_7+\sigma_2\sigma_6\sigma_4\sigma_8$,

$g_{16}=\sigma_1\sigma_3\sigma_6\sigma_8+\sigma_2\sigma_4\sigma_5\sigma_7$,

$g_{17}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6+$--- (8 terms),

$g_{18}=\sigma_1\sigma_2\sigma_3\sigma_5\sigma_6\sigma_7+$--- (4 terms),

$g_{19}=\sigma_1\sigma_2\sigma_3\sigma_5\sigma_7\sigma_8+$--- (4 terms),

$g_{20}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_7+$--- (4 terms),

$g_{21}=\sigma_1\sigma_2\sigma_4\sigma_5\sigma_6\sigma_7+$--- (8 terms),

$g_{22}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7\sigma_8$,

$g_{23}=\sigma_1\sigma_2\sigma_3+$--- (8 terms),

$g_{24}=\sigma_1\sigma_2\sigma_6+$--- (16 terms),

$g_{25}=\sigma_1\sigma_2\sigma_7+$--- (16 terms),

$g_{26}=\sigma_1\sigma_5\sigma_3+$--- (8 terms),

$g_{27}=\sigma_1\sigma_3\sigma_6+$--- (8 terms),

$g_{28}=\sigma_1\sigma_2\sigma_3\sigma_5+$--- (8 terms),

$g_{29}=\sigma_1\sigma_2\sigma_3\sigma_5\sigma_6+$--- (16 terms),

$g_{30}=\sigma_1\sigma_3\sigma_4\sigma_5\sigma_6+$--- (16 terms),

$g_{31}=\sigma_1\sigma_2\sigma_3\sigma_5\sigma_7+$--- (8 terms),

$g_{32}=\sigma_1\sigma_2\sigma_3\sigma_6\sigma_8+$--- (8 terms),

$g_{33}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7+$--- (8 terms), (A15)

Where in order to save space, only one typical term for some invariants is written. Invariants of Eq. (A15) satisfy the relations:

$g_6= g_1^2/2-g_2-g_3-g_4-g_5$

$g_9= g_4g_5-2g_3$

$g_{10}=g_4g_6-2g_2$

$g_{11}=g_3g_5-2g_4$

$g_{12}=g_2g_3-2g_6$

$g_{13}=g_3g_4-2g_5$

$g_{16}= (g_5^2+ g_6^2-4-g_{13}-2g_5-g_4^2-g_2^2-g_3^2)/6$

$g_7=(g_2^2+4g_{16}-g_6^2)/4$

$g_{15}=g_5^2/2-2-g_7-g_{16}$

$g_8=g_3^2/2-2-g_{15}$

$g_{14}=g_4^2/2-2-g_{15}$

$g_{22}=g_7^2/2-1$

$g_i=g_{22}g_{i-15}$ for i=17,---21,

$g_{23}=g_1(2g_2-g_3-g_4+2g_5-g_6-2)/6$

$g_{24}=2g_{23}-g_1(g_2+g_6-2g_5+2g_4)/2,$

$g_{25}=2g_{23}-g_1(g_2-g_6+2g_5-2g_4)/2,$

$g_{26}=-2g_{23}+g_1(g_2-g_6+2g_5-2)/2,$

$g_{29}=g_{23}-g_1(g_2-g_6)/2,$

$g_{i+8} = g_{22} g_{i-5}$ for i = 28, 29, ---32,

$g_{33} = g_{22} g_1$ (A16)

S9 d=3 $\upsilon(\sigma_1, --\sigma_8)$ has the symmetry properties of the primitive unit cell for the FCC lattice. The longest diagonal is in the σ_1, σ_7 direction. For the unit cell of Fig. A3, $|\vec{a}| = |\vec{b}| = |\vec{c}|$, $\alpha = \beta = \gamma = 60^0$.

$g_1 = \sigma_1 + \sigma_7$

$g_2 = \sigma_2 + \sigma_4 + \sigma_5 + \sigma_3 + \sigma_6 + \sigma_8$,

$g_3 = \sigma_2\sigma_4 + \sigma_4\sigma_5 + \sigma_2\sigma_5 + \sigma_3\sigma_6 + \sigma_3\sigma_8 + \sigma_6\sigma_8$,

$g_4 = \sigma_1(\sigma_3 + \sigma_6 + \sigma_8) + \sigma_7 (\sigma_2 + \sigma_4 + \sigma_5)$,

$g_5 = \sigma_2\sigma_8 + \sigma_3\sigma_5 + \sigma_4\sigma_6$,

$g_6 = g_1\sigma_7$,

$g_7 = \sigma_1(\sigma_2 + \sigma_4 + \sigma_5) + \sigma_7(\sigma_3 + \sigma_6 + \sigma_8)$,

$g_8 = \sigma_2\sigma_3 + \sigma_2\sigma_6 + \sigma_5\sigma_6 + \sigma_5\sigma_8 + \sigma_4\sigma_8 + \sigma_3\sigma_4$,

$g_9 = \sigma_1\sigma_2\sigma_3\sigma_4 +$--- (6 terms),

$g_{10} = \sigma_1\sigma_2\sigma_3\sigma_8 +$--- (12 terms),

$g_{11} = \sigma_1\sigma_2\sigma_4\sigma_7 +$--- (6 terms),

$g_{12} = \sigma_2\sigma_3\sigma_6\sigma_8 +$--- (6 terms),

$g_{13} = \sigma_1\sigma_2\sigma_3\sigma_6 +$--- (6 terms),

$g_{14} = \sigma_1\sigma_2\sigma_4\sigma_5 + \sigma_3\sigma_6\sigma_7\sigma_8$,

$g_{15} = \sigma_1\sigma_2\sigma_3\sigma_7 +$--- (6 terms),

$g_{16} = \sigma_2\sigma_3\sigma_4\sigma_8 +$--- (6 terms),

$g_{17} = \sigma_2\sigma_3\sigma_7\sigma_8 +$--- (12 terms),

$g_{18} = \sigma_1\sigma_2\sigma_7\sigma_8 + \sigma_1\sigma_4\sigma_6\sigma_7 + \sigma_1\sigma_5\sigma_3\sigma_7$,

$g_{19} = \sigma_3\sigma_4\sigma_5\sigma_6 + \sigma_2\sigma_3\sigma_5\sigma_8 + \sigma_2\sigma_6\sigma_4\sigma_8$,

$g_{20} = \sigma_1\sigma_3\sigma_6\sigma_8 + \sigma_2\sigma_4\sigma_5\sigma_7$,

$g_{21} = \sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_7 +$--- (6 terms),

$g_{22} = \sigma_1\sigma_2\sigma_3\sigma_4\sigma_6\sigma_8 +$--- (6 terms),

$g_{23}=\sigma_1\sigma_2\sigma_3\sigma_5\sigma_7\sigma_8+\cdots$ (3 terms)

$g_{24}=\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_8$,

$g_{25}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6+\cdots$ (6 terms)

$g_{26}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_6\sigma_7+\cdots$ (6 terms)

$g_{27}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7\sigma_8$

$g_{28}=\sigma_1\sigma_2\sigma_4+\cdots$ (6 terms),

$g_{29}=\sigma_2\sigma_3\sigma_6+\cdots$ (6 terms),

$g_{30}=\sigma_1\sigma_2\sigma_6+\cdots$ (12 terms),

$g_{31}=\sigma_1\sigma_7(\sigma_2+\sigma_4+\sigma_5+\sigma_3+\sigma_6+\sigma_8)$,

$g_{32}=\sigma_1\sigma_2\sigma_8+\cdots$ (6 terms),

$g_{33}=\sigma_2\sigma_6\sigma_8+\cdots$ (12 terms),

$g_{34}=\sigma_1\sigma_3\sigma_6+\cdots$ (6 terms),

$g_{35}=\sigma_3\sigma_6\sigma_8+\sigma_2\sigma_4\sigma_5$,

$g_{36}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5+\cdots$ (6 terms)

$g_{37}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_7+\cdots$ (6 terms)

$g_{38}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_6+\cdots$ (12 terms),

$g_{39}=\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6+\cdots$ (6 terms),

$g_{40}=\sigma_1\sigma_3\sigma_4\sigma_5\sigma_6+\cdots$ (6 terms),

$g_{41}=\sigma_1\sigma_3\sigma_4\sigma_5\sigma_7+\cdots$ (12 terms),

$g_{42}=\sigma_1\sigma_2\sigma_3\sigma_6\sigma_8+\cdots$ (6 terms),

$g_{43}=\sigma_1\sigma_2\sigma_4\sigma_5\sigma_7+\sigma_1\sigma_3\sigma_6\sigma_8\sigma_7$,

$g_{44}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_8+\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7\sigma_8$,

$g_{45}=\sigma_1\sigma_2\sigma_3\sigma_4\sigma_5\sigma_6\sigma_7+\cdots$ (6 terms), (A17)

Where in order to save space, only one typical term for some invariants is written. Invariants of Eq(A15) satisfy the relations:

$g_6=g_1^2/2-1$

$g_7=g_1g_2-g_4$

$g_8=g_2^2/2-3-g_3-g_5$

$g_{10}=g_4g_5-g_7$

$$g_{11}=g_3g_6$$

$$g_{12}=g_3g_5-2g_8$$

$$g_{13}=g_4g_8/2-g_7$$

$$g_{14}=(g_3g_7-2g_7-g_{13}-g_{10})/3$$

$$g_{15}=g_6g_8$$

$$g_{18}=g_5g_6,$$

$$g_{19}=(g_5^2-3)/2,$$

$$g_{16}=g_3^2/2-3-g_3-g_{19},$$

$$g_{17}=(g_7+g_8)\ (g_5+g_6)-2(g_3+g_4)-g_{15}-g_{16},$$

$$g_9=g_7g_8/2-g_4-g_{17}/2,$$

$$g_{20}=(g_3g_4-2g_4-g_{17}-g_9)/3,$$

$$g_{29}=g_{20}^2/2-1,$$

$$g_i=g_{27}g_{i-18} \quad \text{for } i=21,22, \ldots 26,$$

$$g_{30}=g_1g_8,$$

$$g_{31}=g_2g_6,$$

$$g_{32}=g_1g_5,$$

$$g_{33}=g_2g_5-g_2,$$

$$g_{34}=(g_2g_4-3g_1-g_{30}-g_{32})/2$$

$$g_{28}=g_1g_3-g_{34}$$

$$g_{29}=g_2g_8-2g_2-g_{33}-g_{28}$$

$$g_{35}=(g_2g_3-2g_2-g_{29}-g_{33})/3,$$

$$g_i=g_{27}\ g_{i-8} \quad \text{for } i = 36, 37, \ldots 45. \qquad \text{(A18)}$$

APPENDIX B

Details of the Calculation

In this Appendix, we outline some techniques used in our computer program to obtain the numerical results. Our computer program can be applied to all systems listed in Appendix A with space dimension and symmetry properties as input parameters. The important programming techniques are as follows:

1. Generation of all possible spin configurations. Let z denote the number of spins on a hypercube unit cell of the d dimensional lattice and NCF denote the number of all possible configuration of such z spins σ_1,--σ_z, then $Z=2^d$, $NCF=2^Z$. Let I be an integer running from o to NCF-1. We express I as a z digit binary number and let 1 correspond to spin up (+1) and 0 correspond spin down (-1), then each integer from 0 to NCF-1 correspond to one spin cofiguration where integer 0 corresponds to all spin down configuration and NCF-1 correspond to all spin up configuration which is the ground state of the ferromagnetic system. Thus, with d as input parameter, we can generate all possible spin configurations.

2. Classification of spin configurations. From Table A1, it is clear that for space dimension $d\geq 2$ there are some systems with different symmetry properties. Thus, for each spin configuration generated in the manner described above, we calculate the values of the basic invariants based on the parameter "sym" and then classify these spin configurations into different degeneracy groups such that the configurations in the same group have the same values for all basic invariants (and hence cell potential) and in different groups have at least one different value. We label the degeneracy group in such a way that the ground state configuration, which is all spin up configuration for ferromagnetic system, belongs to the final group. For each group, we also store the degeneracy Di (ie the number

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of configurations in the group) and the configurations belonging to this group. We will use $\vec{D}$ to denote the vector whose elements are degeneracy, ie $\vec{D}=(D_1,D_2,---D_{\ell+1})$.

3. Calculation of the column vector $T^{-1}\vec{C}$.

In this section, we will derive formulas for the vector $T^{-1}\vec{C}$ which appears at the end of Eq. (17) and (18). From Eq. (5b), it is easy to show that

$$K_o^{(\alpha)}=\frac{1}{NCF}\sum_{i=1}^{\ell+1} v_i^{(\alpha)} Di. \qquad (B1)$$

Thus, Eq (13) may be rewritten as:

$$f^{(\alpha)}= - 1/Z^{\alpha}(1/NCF \sum_{i=1}^{\ell+1} \upsilon_i^{(\alpha)} Di+1n2) \qquad (B2a)$$

for $T>T_c$ and

$$f^{(\alpha)}= - 1/Z^{\alpha} (\upsilon^{(\alpha)}_{\ell+1} + 1n\ 2)$$

for $T<T_c$, where $\upsilon^{(\alpha)}_{\ell+1}$ is the ground state cell potential. We now take the first derivative of Eq (B2) with respect to q. By the chain rule, it is easy to show that:

$$\frac{\delta f^{(\alpha)}}{\delta q} = \frac{\delta\vec{\upsilon}0}{\delta q}\cdot\frac{\delta\vec{\upsilon}1}{\delta\vec{\upsilon}0}\cdot\cdots\cdot\frac{\delta\vec{\upsilon}^{(m)}}{\delta\vec{\upsilon}^{(m-1)}}\cdots\frac{\delta\vec{\upsilon}^{(\alpha)}}{\delta\vec{\upsilon}^{(\alpha-1)}}\ 1/Z^{\alpha}\ \vec{C}_o, \qquad (B3)$$

where

$$\vec{C}_o=(D_1,D_2,---D_{\ell+1})\equiv\vec{D} \qquad (B4a)$$

for $T>T_c$ and

$$\vec{C}_o=(0\ ,\ 0\ ,\ -----,\ 0,\ 1) \qquad (B4b)$$

for $T<T_c$. Comparing Eq (17) and (B3), it is obvious that $T^{-1}\vec{C}$ of Eq (17) is jsut $\vec{C}_o$ of Eq (B3) and (B4).

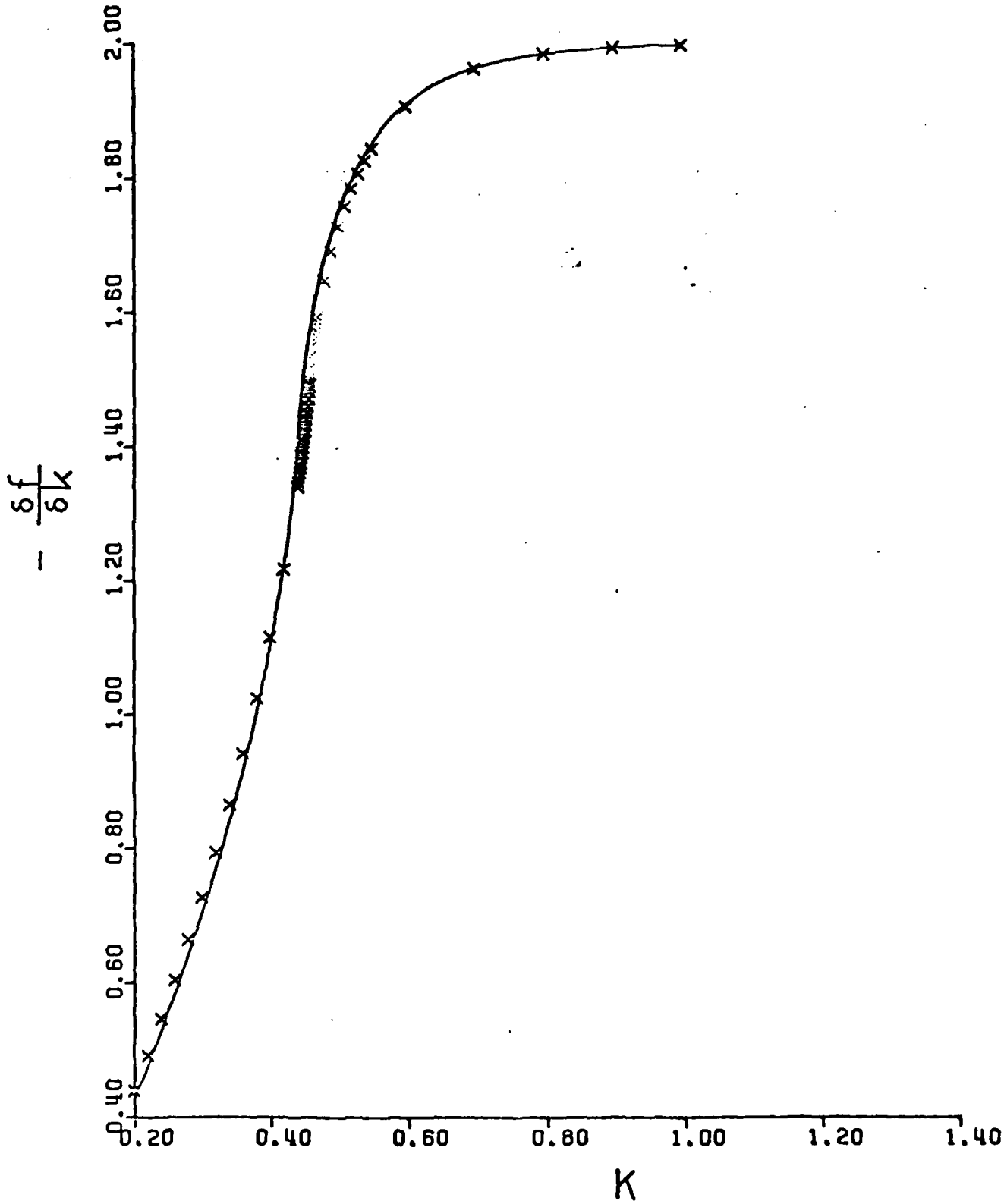

$-\frac{\delta f}{\delta K}$
2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.40
0.60
0.80
1.00
1.20
1.40
K

Fig 1a

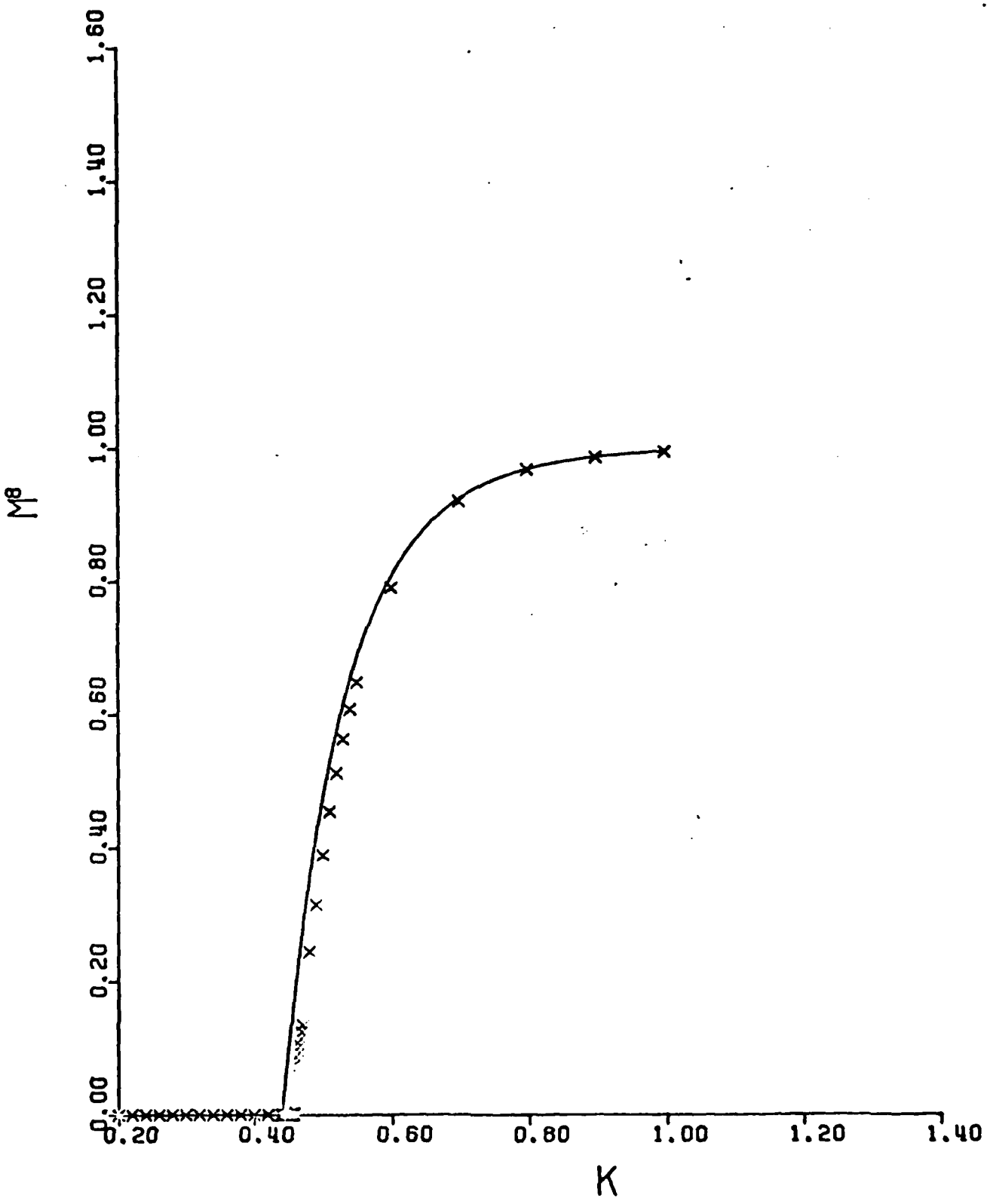
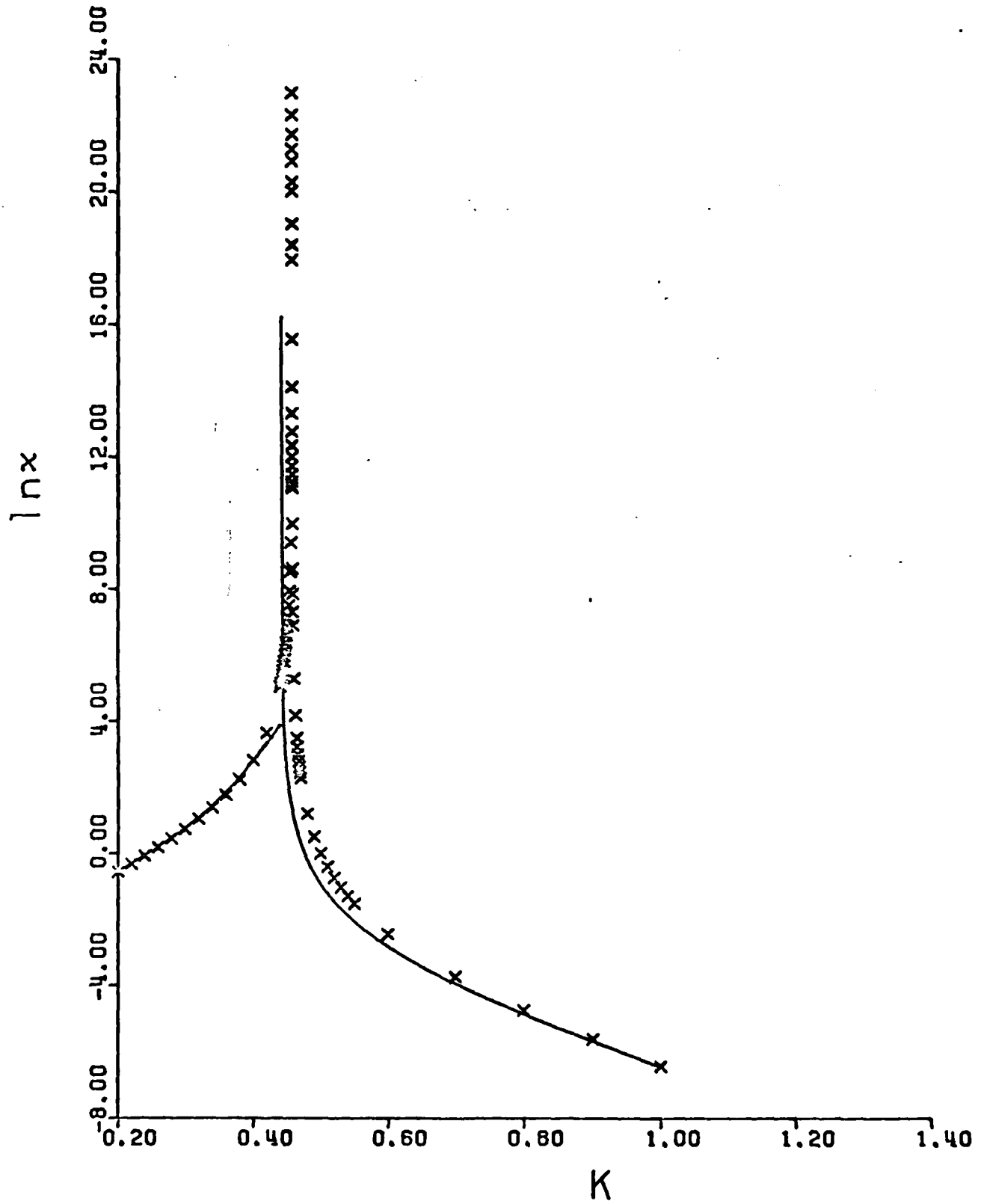

1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
M^B
0.20
0.40
0.60
0.80
1.00
1.20
1.40
K

Fig 1C


lnx
24.00
20.00
16.00
12.00
8.00
4.00
0.00
-4.00
-8.00
0.20
0.40
0.60
0.80
1.00
1.20
1.40
K

Fg 1d

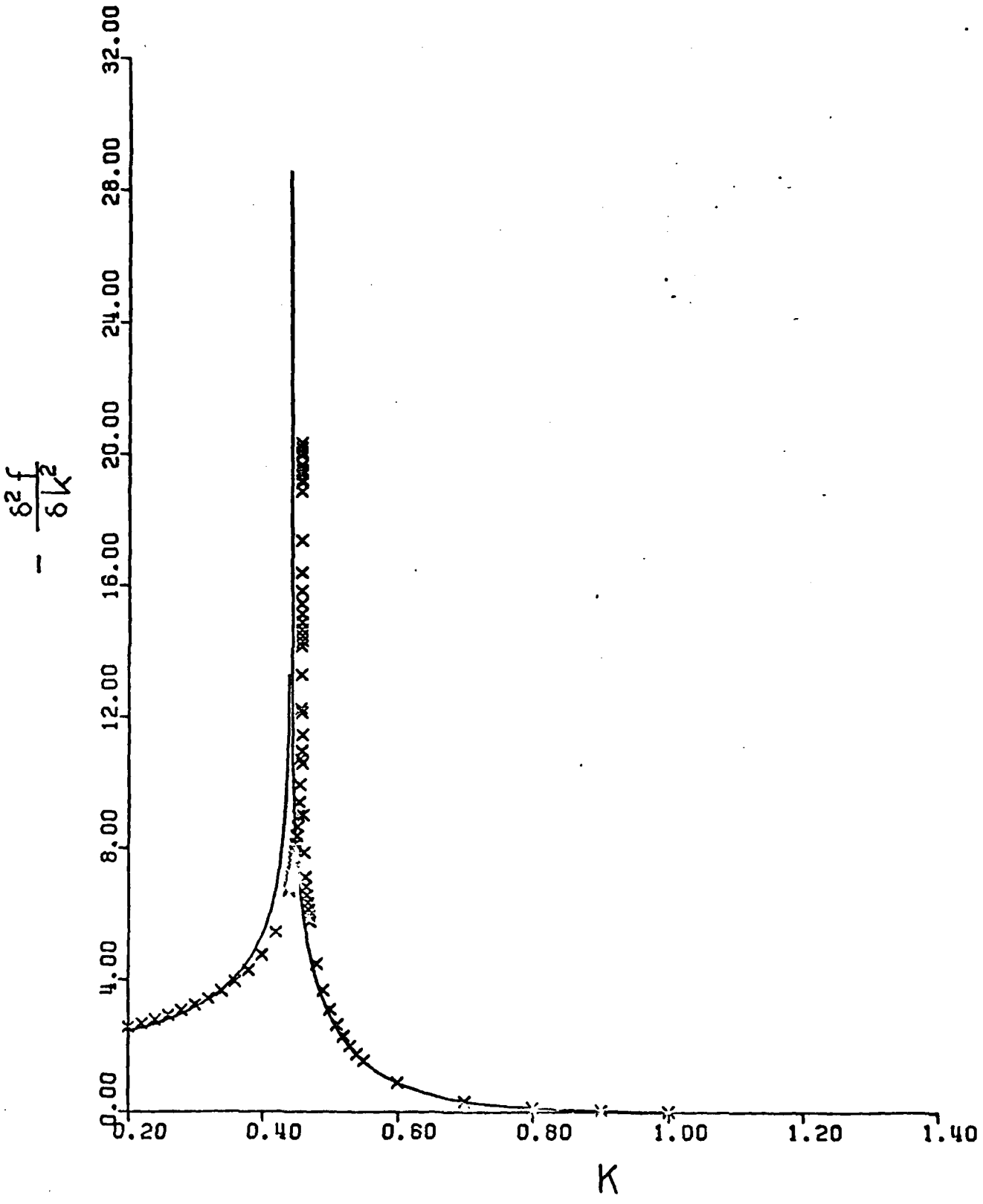

$-\frac{\delta^2 f}{\delta k^2}$
32.00
28.00
24.00
20.00
16.00
12.00
8.00
4.00
0.00
0.20
0.40
0.60
0.80
1.00
1.20
1.40
K

Fig 1b

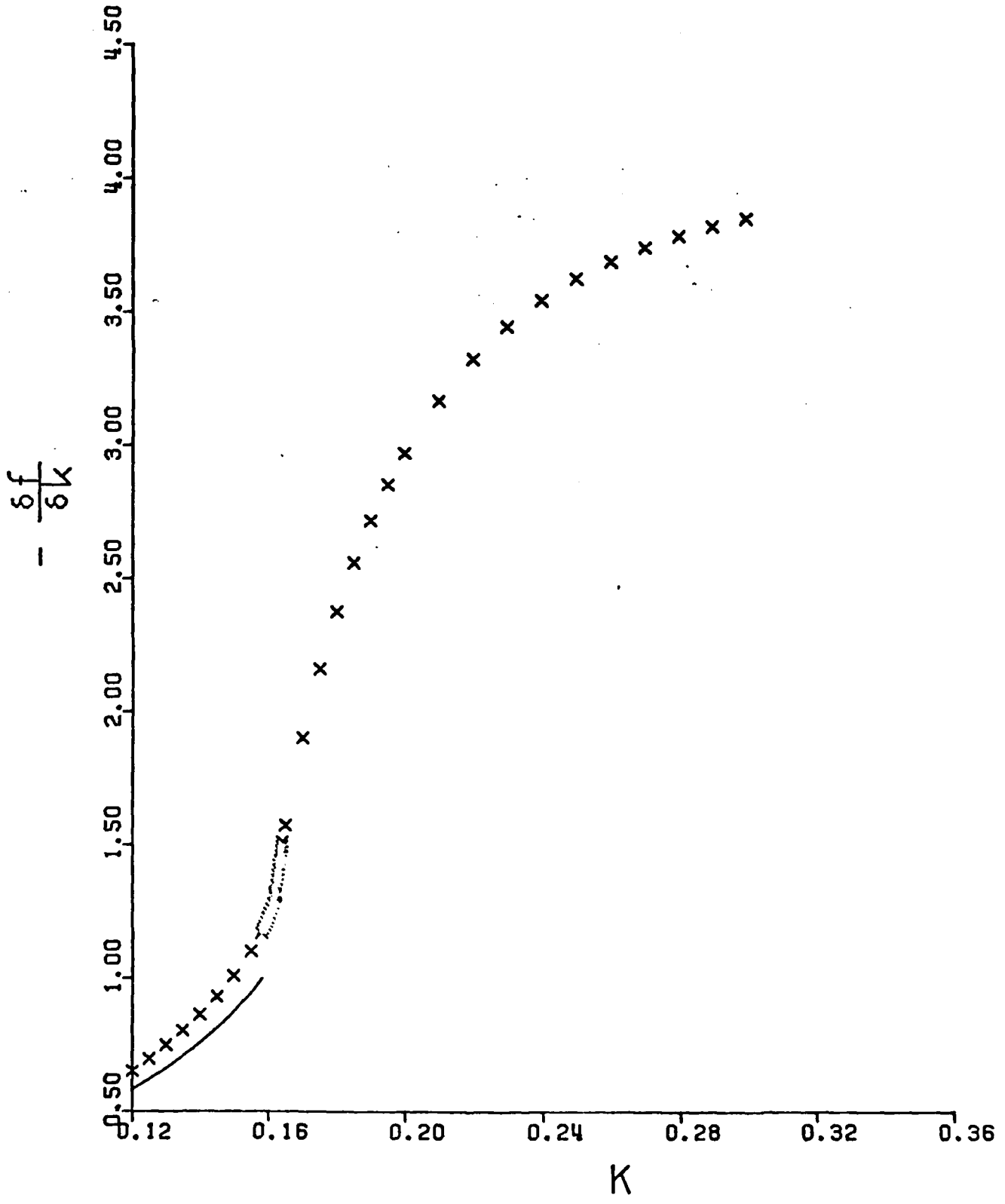

$-\frac{\delta f}{\delta K}$
0.50
1.00
1.50
2.00
2.50
3.00
3.50
4.00
4.50
0.12
0.16
0.20
0.24
0.28
0.32
0.36
K

Fig 3

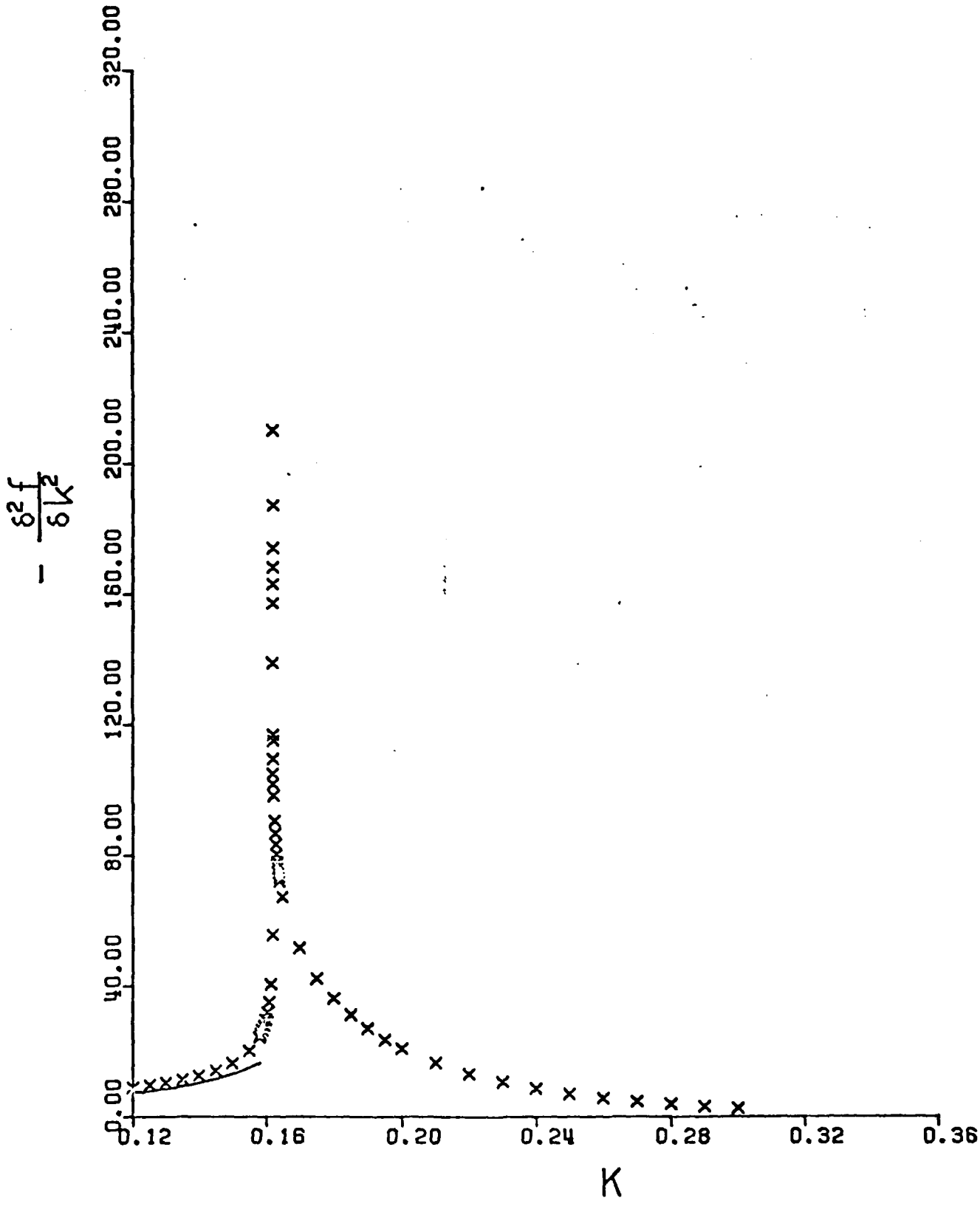

$-\frac{\delta^2 f}{\delta K^2}$
320.00
280.00
240.00
200.00
160.00
120.00
80.00
40.00
0.00
0.12
0.16
0.20
0.24
0.28
0.32
0.36
K

Fig 2b

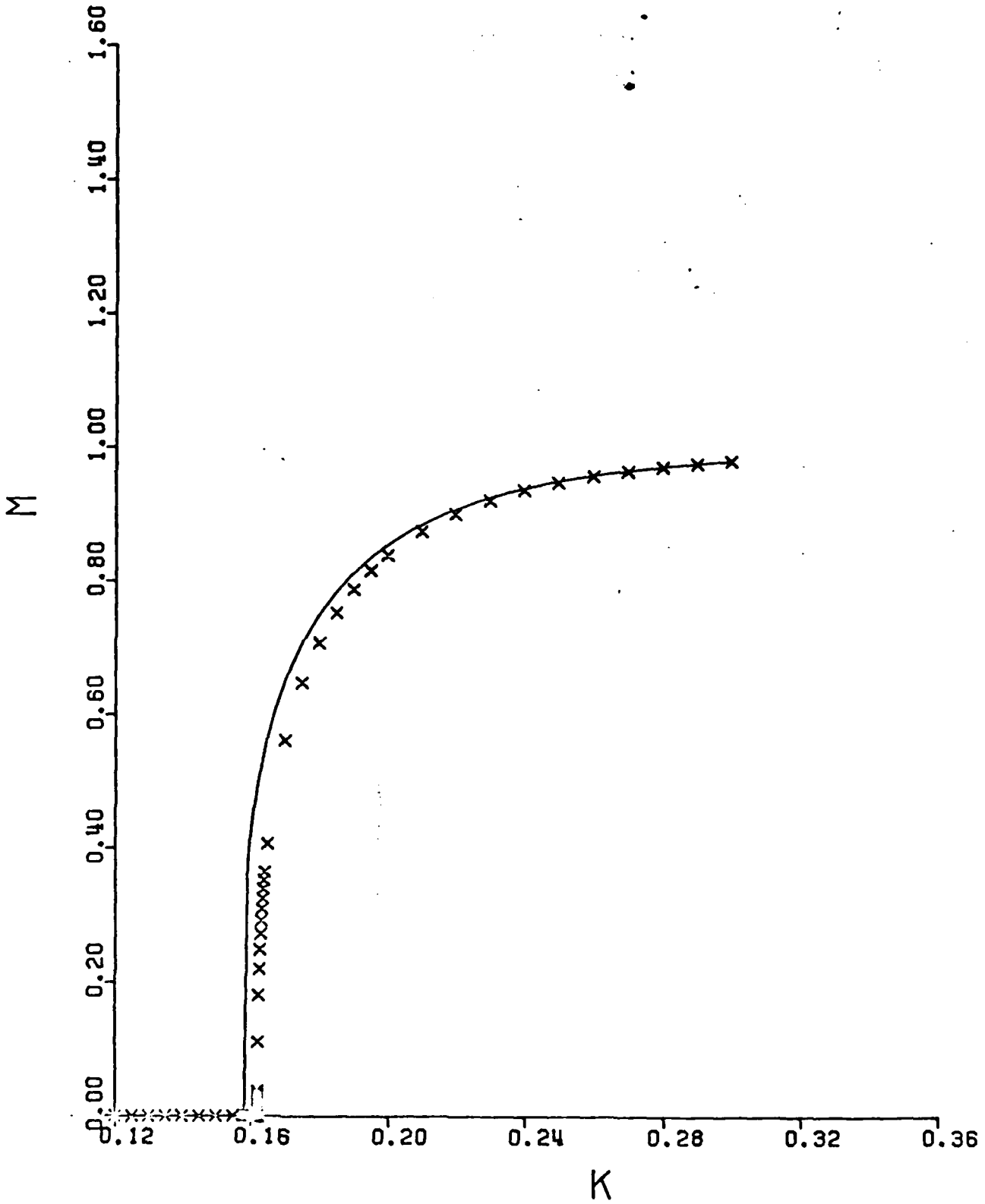

M
1.60
1.40
1.20
1.00
0.80
0.60
0.40
0.20
0.00
0.12
0.16
0.20
0.24
0.28
0.32
0.36
K

Fig. C

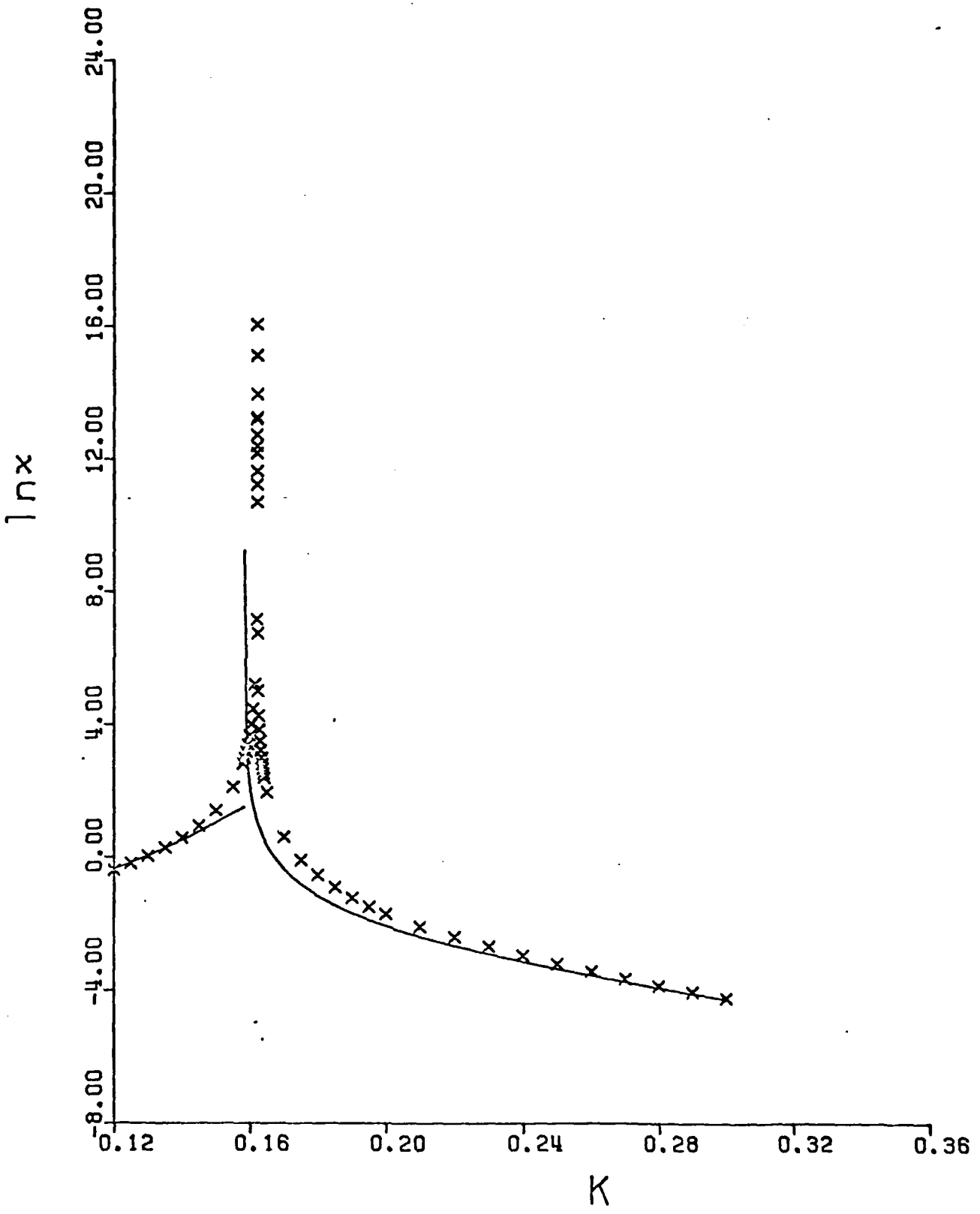

lnx
24.00
20.00
16.00
12.00
8.00
4.00
0.00
-4.00
-8.00
0.12
0.16
0.20
0.24
0.28
0.32
0.36
K

Fig 2 d

Fig A1

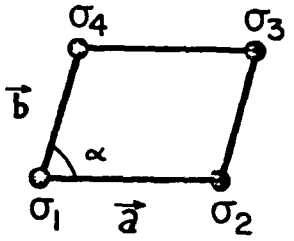


Fig A2

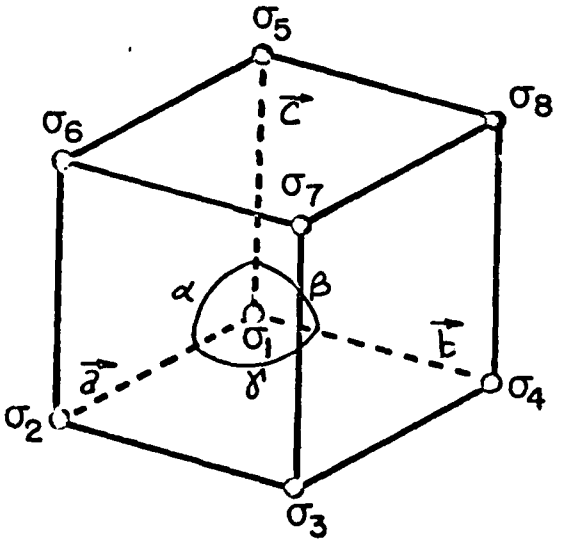


Fig A3


DA
FIL